Butyl 3-methoxypropionate 4195-88-4 | DTXSID30194709

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Mode	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)	Test (25%	Test (25%)		
Q2	RMSE	R2	RMSE	R2	RMSE		
0.87	0.81	0.87	0.82	0.86	0.86		

Model Results

Predicted value: 6.04e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 9.17e-01

Confidence level: 7.02e-01

Nearest Neighbors from the Training Set

Image not found

Butyl 3-methoxypropionate

Measured: 6.12e-02 Predicted: 6.04e-02

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Methyl 3-butoxypropanoate

Measured: 5.12e-02 Predicted: 5.88e-02

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2-Butoxyethyl acetate Measured: 5.62e-02 Predicted: 6.06e-02

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propyl 3-propoxypropanoate

Measured: 2.07e-02 Predicted: 3.66e-02